

Magnetic hyperfine structure of the ground-state doublet in highly charged ions $^{229}\text{Th}^{89+,87+}$ and the Bohr-Weisskopf effect

E. V. Tkalya^{1,2,3,*} and A. V. Nikolaev¹

¹*Skobeltsyn Institute of Nuclear Physics Lomonosov Moscow State University, Leninskie gory, Moscow 119991, Russia*

²*Nuclear Safety Institute of RAS, Bol'shaya Tulkaya 52, Moscow 115191, Russia*

³*National Research Nuclear University MEPhI, 115409, Kashirskoe shosse 31, Moscow, Russia*

(Dated: June 24, 2016)

The magnetic hyperfine (MHF) structure of the $5/2^+(0.0 \text{ eV})$ ground state and the low-lying $3/2^+(7.8 \text{ eV})$ isomeric state of the ^{229}Th nucleus in highly charged ions Th^{89+} and Th^{87+} is calculated. The distribution of the nuclear magnetization (the Bohr-Weisskopf effect) is accounted for in the framework of the collective nuclear model with the wave functions of the Nilsson model for the unpaired neutron. The deviations of the MHF structure for the ground and isomeric states from their values in the model of point-like nuclear magnetic dipole are calculated. The influence of the mixing of the states with the same quantum number F on the energy of sublevels is studied. Taking into account the mixing of states, the probabilities of the transitions between the components of MHF structure are found.

PACS numbers: 32.10.Fn, 27.90.+b, 31.15.ve

I. INTRODUCTION

The low lying $3/2^+(7.8 \pm 0.5 \text{ eV})$ state [1, 2] of the ^{229}Th nucleus has been the subject of intense experimental [1–16] and theoretical research [17–34] in the past decades. The interest is caused by new possibilities which are emerging in the study of such unusual nuclear level. The works on this problem are multidisciplinary, including fields of science as diverse as nuclear physics, solid state physics, atomic physics, optics and laser physics. Three excellent experiments, Refs. [1, 4, 16], which gave us the knowledge on the existence of the low-lying isomeric state and provided with estimations of its energy, demonstrate the variety of experimental methods needed for the characterization of this state. The experimental technique gradually evolves from traditional methods of nuclear spectroscopy [1, 3, 4] to those used in low energy physics: solid state physics, optics, etc. [13–16].

In a number of theoretical publications authors have drawn attention to exciting possibilities related with the existence of the $3/2^+(7.8 \pm 0.5 \text{ eV})$ state and its decay channels. Here one can mention a refinement of some fundamental laws and symmetries of Nature, for example, the CP-violation, the variation of the fine structure constant [28, 29, 35–37], the local Lorentz invariance and the Einstein equivalence principle [38]. Unusual for traditional nuclear physics decay channels of the isomeric state – the electron bridge [17, 39] and nuclear light [25–27] – probably imply that the $3/2^+(7.8 \pm 0.5 \text{ eV})$ state can be occupied by laser emission through nuclear photo-excitation process [20, 27] or inverse electron bridge [20, 40, 41]. An interesting consequence of such excitations is the detection of the α -decay of the isomeric state [21] with the possibility of checking the ex-

ponentiality of the decay law of an isolated metastable state at long times [24]. Finally, we should mention two important technological applications – the nuclear clock [12, 42–44], and the gamma-ray laser of the optical range [31, 45], both of which can lead to a breakthrough in their fields.

In the present study we have carried out calculations and give numerical estimations for the position of the sublevels of the $5/2^+(0.0)$ and $3/2^+(7.8 \text{ eV})$ states in the highly charged ions $^{229}\text{Th}^{89+}$ and $^{229}\text{Th}^{87+}$. The Th^{89+} ion has one electron which occupies the $1s_{1/2}$ electron shell, while the Th^{87+} ion has three electrons on the $1s_{1/2}$ and $2s_{1/2}$ electron shells, i.e. the $(1s_{1/2})^2(2s_{1/2})^1$ electron configuration. We have taken into account the Bohr-Weisskopf effect and the mixing of the states, and calculated the probabilities of the transitions between the sublevels.

Our calculations can be instrumental in experimental studies of the magnetic hyperfine (MHF) interaction in highly ionized atoms investigated in a storage ring of accelerator complex [46–49].

II. MAGNETIC HYPERFINE INTERACTION

A preliminary (and as a rule, overestimated) estimation of the MHF interaction can be obtained by using the Fermi contact interaction [50].

The electron in the $1s_{1/2}$ state of the $^{229}\text{Th}^{89+}$ ion or electron in the $2s_{1/2}$ state of the $^{229}\text{Th}^{87+}$ ion result in a strong magnetic field at the center of the ^{229}Th nucleus [19, 22]. The value of this field is given by the formula for the Fermi contact interaction (see in [50])

$$\mathbf{H} = -\frac{16\pi}{3}\mu_B\frac{\boldsymbol{\sigma}}{2}|\psi_e(0)|^2, \quad (1)$$

where $\mu_B = e/2m$ is the Bohr magneton, e is the electron charge, m is the electron mass, $\boldsymbol{\sigma}$ are the Pauli matrixes,

*Electronic address: tkalya@srd.sinp.msu.ru

and $\psi_e(0)$ is the amplitude of the electron wave function at the origin.

The interaction of the point magnetic moment of the ground state ($\mu_{gr} = 0.45$) or the isomeric state ($\mu_{is} = -0.076$) of the ^{229}Th nucleus with the magnetic field (1) leads to a splitting of the nuclear levels. The energy of the sublevels is determined by the formula

$$E = E_{int} \frac{F(F+1) - I(I+1) - s(s+1)}{2Is}, \quad (2)$$

with the interaction energy

$$E_{int} = -\mu_{gr(is)} \mu_N H. \quad (3)$$

Here $\mu_N = e/2M_p$ is the nuclear magneton (M_p is the proton mass), I stands for the nuclear spin, s is the electron spin. The quantum number F takes two values $F = I \pm 1/2$ for both the ground and isomeric state.

To obtain the magnetic field and the hyperfine splittings one has to find the amplitude of the electron wave function at the nucleus, $\psi_e(0)$, Eq. (1). The details of the calculations of $\psi_e(0)$ are given in the next section. For precise determination of $\psi_e(0)$ the calculations should be self-consistent, relativistic and take into account the finite size of the nucleus.

III. CALCULATION OF ELECTRON WAVE FUNCTIONS

In the present work, the wave function $\psi_{1s_{1/2}}(x)$ of the electron in the $(1s_{1/2})^1$ configuration has been found numerically by solving the Dirac equation in the Coulomb potential of the nucleus with the radius $R_0 = 1.2 A^{1/3}$ fm (where A is the atomic number). The nucleus has been considered spherical with the homogeneous positive charge distribution. In this case the electron potential energy in the units of the electron mass is given by

$$V(x) = \begin{cases} \frac{1}{2} \frac{e^2 Z}{m R_0} (3 - x^2), & x \leq 1 \\ \frac{e^2 Z}{m R_0} \frac{1}{x}, & x > 1 \end{cases} \quad (4)$$

Here $x = r/R_0$, where r is the modulus of the electron radius vector \mathbf{r} , Z is the nuclear charge ($Z = 90$ for Th). The large (g) and small (f) radial components of the electron wave function $\psi_e(x)$ are found from the system

$$\begin{aligned} xg'(x) - b(E + 1 - V(x))xf(x) &= 0, \\ xf'(x) + 2f(x) + b(E - 1 - V(x))xg(x) &= 0, \end{aligned} \quad (5)$$

where $b = mR_0$. The electron wave function is normalized by the condition $\int_0^\infty (g^2(x) + f^2(x))x^2 dx = 1$.

In the following we work with the variable $x = r/R_0$ instead of $x = r/a_B$, where a_B is the Bohr radius, commonly used in atomic physics because for calculations of the Bohr-Weisskopf effect we need a nuclear scale. However, when necessary we will return to atomic units and give the values of the electron wave functions in units of $a_B^{3/2}$ to compare with the calculations of other authors.

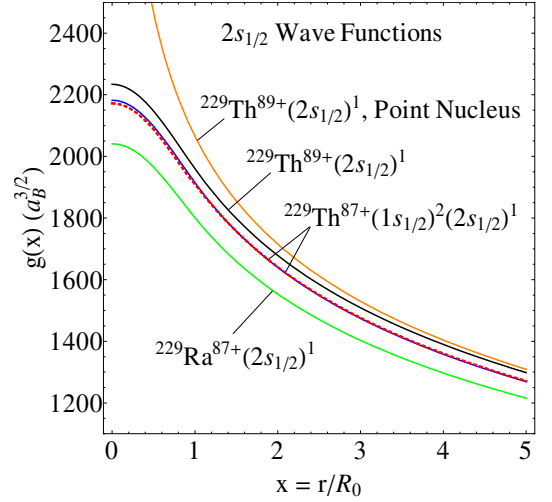


Figure 1: (color online). The large radial component $g(x)$ of the $2s_{1/2}$ state (in a.u.) calculated in various models (see text for details). $^{229}\text{Th}^{89+}(2s_{1/2})^1$ is the hydrogen-like ion model for the $2s_{1/2}$ state (i.e. the model without screening). $^{229}\text{Ra}^{87+}(2s_{1/2})^1$ stands for the full screening of the nuclear charge +2 by two electrons in the $1s_{1/2}$ state. $^{229}\text{Th}^{87+}(1s_{1/2})^2(2s_{1/2})^1$, full line: the potential from two electrons in the $1s_{1/2}$ state is added to the nuclear potential. $^{229}\text{Th}^{87+}(1s_{1/2})^2(2s_{1/2})^1$, dashed line: *ab initio* DFT calculation [51, 52]

The calculation of the Bohr-Weisskopf effect for the $2s_{1/2}$ electron state in the $(1s_{1/2})^2(2s_{1/2})^1$ three electron configuration has been performed by three different methods, Fig. 1.

At first, we have found the upper and lower boundaries for the $2s_{1/2}$ electron wave function. For this purpose we have used the wave function of the $2s_{1/2}$ state obtained in the field of the hydrogen-like ion. As the hydrogen-like ion we take (i) the $^{229}\text{Th}^{89+}$ ion with $Z = 90$ and (ii) the $^{229}\text{Ra}^{87+}$ ion. In the last case we have assumed that two electrons in the $1s_{1/2}$ state perfectly screen the nuclear charge +2, and $Z = 90 - 2 = 88$.

In the second model we have used a more sophisticated approach by adding to the nuclear potential (4) the Coulomb contribution from the electron density of two electrons in the $1s_{1/2}$ state. The shortcoming of this calculation is that it does not take into account the interaction between electrons in the $1s_{1/2}$ state and between electrons in the $1s_{1/2}$ and $2s_{1/2}$ states.

Finally, we have carried out *ab initio* numerical calculations inside and outside the nuclear region within the density functional method (DFT) taking the full account of the electron self-consistent field by employing the atomic part of the code [51, 52]. The precise atomic DFT calculations have been performed with two main variants for the exchange correlation potential and energy. The first functional belongs to the local density approximation (LDA) [53, 54], while the second to the generalized gradient approximation (GGA) of Perdew,

Burke, and Ernzerhof (PBE) [55, 56]. Both variants represent standard choices within the DFT method.

As follows from Fig. 1 the refined calculation of the large component $g_{2s_{1/2}}(x)$ of the $2s_{1/2}$ state practically coincides with the calculation in the second model with the additional potential created by the two noninteracting $1s_{1/2}$ electrons. Moreover, for some estimations of the magnetic field and MHF interaction one can use the simple calculation in the hydrogen-like ion model for $^{229}\text{Th}^{89+}(2s_{1/2})^1$. The difference in the amplitude of the $2s_{1/2}$ large component at nucleus, $g_{2s_{1/2}}(0)$, for the $(2s_{1/2})^1$ configuration in $^{229}\text{Th}^{89+}$ and for the $(1s_{1/2})^2(2s_{1/2})^1$ configuration in $^{229}\text{Th}^{87+}$ amounts to 2.5%. For many applications this difference is not essential.

To evaluate the magnetic field one can use Eq. (1) with $\psi_e(0) = Y_{00}(\vartheta, \varphi)g(0)/R_0^{3/2}$, where $Y_{00} = 1/\sqrt{4\pi}$ is the spherical harmonic with $l = m = 0$ describing the angular part of the s -states. (Notice that for s -states $f(x=0) = 0$.) We have $g_{1s_{1/2}}(0) = 8.46 \times 10^{-3}$ for the $(1s_{1/2})^1$ configuration in the $^{229}\text{Th}^{89+}$ ion and $g_{2s_{1/2}}(0) = 3.57 \times 10^{-3}$ for the $2s_{1/2}$ state in the $(1s_{1/2})^2(2s_{1/2})^1$ configuration of the $^{229}\text{Th}^{87+}$ ion according to the *ab initio* calculations. Now by means of Eq. (1) we obtain 112 MT for the magnetic field at the ^{229}Th nucleus of the $^{229}\text{Th}^{89+}$ ion and 20 MT for the magnetic field of the $^{229}\text{Th}^{87+}$ ion.

Notice that in the atomic units $\psi_e(0) = Y_{00}(\vartheta, \varphi)g(0)/a_B^{3/2}$, where $g_{1s_{1/2}}(0) = 5.18 \times 10^3$, and $g_{2s_{1/2}}(0) = 2.18 \times 10^3$.

IV. THE BOHR-WEISSKOPF EFFECT

The influence of the finite nuclear size on the hyperfine splitting was first considered by Bohr and Weisskopf [57]. Later the effect of the distribution of nuclear magnetization on hyperfine structure in muonic atoms was studied by Le Bellac [58]. According to their works, the energy of sublevels of a deformed nucleus is given by Eq. (2), where

$$E_{int} = \int d^3r \mathbf{j}(\mathbf{r}) \mathbf{A}(\mathbf{r}), \quad (6)$$

is the energy of the interaction of the electron current $\mathbf{j}(\mathbf{r}) = -e\psi_e^\dagger(\mathbf{r})\boldsymbol{\alpha}\psi_e(\mathbf{r})$ ($\boldsymbol{\alpha} = \gamma^0\boldsymbol{\gamma}$, γ are the Dirac matrices) with the vector potential of the electromagnetic field $\mathbf{A}(\mathbf{r})$ generated by the magnetic moment of the nucleus.

For a system of “rotating deformed core (with the collective rotating angular momentum \mathfrak{R}) + unpaired neutron (with the spin \mathbf{S}_n)”, the vector-potential is determined by the relation [57, 58]

$$\mathbf{A}(\mathbf{r}) = - \int d^3R [\rho_n(\mathbf{R})g_S\mathbf{S}_n + \rho_{core}^m(\mathbf{R})g_R\mathfrak{R}] \times \nabla_r \frac{1}{|\mathbf{r} - \mathbf{R}|}, \quad (7)$$

where $\rho_n(\mathbf{R})$ is the distribution of the spin part of the nuclear moment and $\rho_{core}^m(\mathbf{R})$ is the distribution of the core magnetization, g_S is the spin g -factor, and g_R is the core gyromagnetic ratio. The distributions $\rho_n(\mathbf{R})$ and $\rho_{core}^m(\mathbf{R})$ are normalized by the conditions $\int d^3R \rho_n(\mathbf{R}) = 1$, $\int d^3R \rho_{core}^m(\mathbf{R}) = 1$.

As follows from Eqs. (6–7), E_{int} consists of two parts, $E_{int} = E_{int}^{(n)} + E_{int}^{(core)}$. Here $E_{int}^{(n)}$ is the energy of the electron interacting with an external unpaired neutron and $E_{int}^{(core)}$ is the energy of the electron interacting with the rotating charged nuclear core. These energies are calculated in accordance with formulas from [58]. In our case the electron interacts with the nucleus in the head levels of rotational bands (for such states we have $K = I$, where K is the component of I along the symmetry axis of the nucleus), and two contributions are given by

$$E_{int}^{(n)} = -\frac{2e^2M_p}{3(M_pR_0)^2}g_K\frac{I^2}{I+1}\left[\int_0^\infty f(x)g(x)dx - \int \varphi_K^*(\mathbf{y})\varphi_K(\mathbf{y})d^3y \int_0^y \left(1 - x^3\frac{2I+1}{I(2I+3)} \times \sqrt{\frac{4\pi}{5}}Y_{20}(\theta)\right) f(x)g(x)dx\right], \quad (8)$$

$$E_{int}^{(core)} = -\frac{2e^2M_p}{3(M_pR_0)^2}g_R\frac{I}{I+1}\left[\int_0^\infty f(x)g(x)dx - \int \rho_{core}^m(\mathbf{y})d^3y \int_0^y (1 - x^3)f(x)g(x)dx\right]. \quad (9)$$

Here, $\varphi_K(\mathbf{R})$ is the wave function of the external neutron (see below), g_K is the intrinsic g factor, $\mathbf{y} = \mathbf{R}/R_0$, \mathbf{R} is the radius vector of the unpaired neutron, and $\rho_{core}^m(\mathbf{y})$ is the normalized nuclear magnetic moment. In the present approach we consider the homogeneous positive charge distribution inside the nuclear sphere, which results in

$$\rho_{core}^m(\mathbf{y}) = \frac{5}{2} \frac{1}{4\pi R_0^3/3} y^2 \sin^2 \theta.$$

We conclude this section by noting that the first term in the square brackets of Eqs. (8) and (9), $\int_0^\infty f(x)g(x)dx$, corresponds to the interaction of the electron with a point nuclear magnetic dipole. The model of the electron interacting with the point nuclear magnetic dipole gives much more precise value of the hyperfine interaction than the Fermi contact interaction, Eqs. (1) and (3).

V. NUCLEAR WAVE FUNCTIONS

For calculations of the nuclear part in Eqs. (8)–(9) we use the standard nuclear wave function [59]

$$\Psi_{MK}^I = \sqrt{\frac{2I+1}{8\pi^2}} D_{MK}^I(\boldsymbol{\Omega}) \varphi_K(\mathbf{R}), \quad (10)$$

where $D_{MK}^I(\mathbf{\Omega})$ is the Wigner D -function [60], $\mathbf{\Omega}$ stands for the three Euler angles, $\varphi_K(\mathbf{R})$ is the wave function of the external neutron coupled to the core, and M is the component of I along the direction of magnetic field.

The wave functions φ_K of the unpaired neutron is taken from the Nilsson model. The structure of the ^{229}Th ground state $5/2^+(0.0)$ is $K^\pi[Nn_z\Lambda] = 5/2^+[633]$. The structure of the isomeric state $3/2^+(7.8 \text{ eV})$ is $3/2^+[631]$ [4]. For each of these states, the wave function has the form

$$\varphi_K = \phi_\Lambda(\varphi)\phi_{\Lambda,n_r}(\eta)\phi_{n_z}(\zeta) \quad (11)$$

where the quantum number $n_r = (N - n_z - \Lambda)/2$, $\zeta = R_0\sqrt{M_p\omega_z}y\cos\theta$ and $\eta = R_0\sqrt{M_p\omega_\perp}y\sin\theta$ are new variables. Here we have introduced new frequencies $\omega_z = \omega_0\sqrt{1+2\delta/3}$ and $\omega_\perp = \omega_0\sqrt{1-4\delta/3}$, where $\omega_0 = 41/A^{1/3} \text{ MeV}$ is the harmonic oscillator frequency, $\delta = 0.95\beta$, and β is the parameter of the nuclear deformation defined by $R = R_0(1 + \beta Y_{20}(\theta) + \dots)$.

For the wave function components we then obtain:

$$\begin{aligned} \phi_\Lambda(\varphi) &= \frac{1}{\sqrt{2\pi}}e^{i\Lambda\varphi}, \\ \phi_{\Lambda,n_r}(\eta) &= \frac{1}{N_\eta}e^{-\eta^2/2}\eta^\Lambda L_{n_r}^{(\Lambda)}(\eta^2), \\ \phi_{n_z}(\zeta) &= \frac{1}{N_\zeta}e^{-\zeta^2/2}H_{n_z}(\zeta), \end{aligned}$$

where $L_{n_r}^{(\Lambda)}$ is the generalized Laguerre polynomial, H_{n_z} is the Hermite polynomial [61], $N_{\eta,\zeta}$ are the normalization factors. In our numerical calculations we took into account the asymmetry of the nucleon wave functions in Eq. (8), but neglected the small difference between ω_z and ω_\perp .

VI. MAGNETIC HYPERFINE STRUCTURE AND MIXING OF SUBLEVELS

The energies of the sublevels calculated according to Eqs. (2), (8)-(9) are given in Tables I – II, third columns. We observe that for the $^{229}\text{Th}^{89+,87+}$ ions there is a reduction of the MHF splitting in comparison with the model of point nucleus. The reduction is 3% for the $5/2^+(0.0)$ ground state and approximately 6% for the $3/2^+(7.8 \text{ eV})$ isomeric state. The difference can be explained by the following: The magnetic field produced by the spin of the nucleon is sensitive to the non-sphericity of the wave functions φ_K . This leads to the appearance of the additional averaging over the angle θ in Eq. (8) [57, 58]. Averaging over the angles reduces the spin contribution with respect to the orbital part. A small imbalance emerged in the system leads to some violation of the “fine tuning” between the spin and orbital parts of the magnetic moment. The relative imbalance is larger for the isomeric state because its magnetic moment smaller than the magnetic moment of the ground state.

Table I: Magnetic hyperfine splitting in the $^{229}\text{Th}^{89+}$ ion. The energy of the sublevels is in eV.

State I^π, F	Point nuclear magnetic dipole	Distributed nuclear magnetic dipole	
		Eqs. (8)-(9) of the present work	Mixing of the $F = 2$ levels
$5/2^+, 3$	0.373	0.362	0.362
$5/2^+, 2$	-0.522	-0.507	-0.526
$3/2^+, 2$	$E_{is} - 0.063$	$E_{is} - 0.059$	$E_{is} - 0.040$
$3/2^+, 1$	$E_{is} + 0.105$	$E_{is} + 0.098$	$E_{is} + 0.098$

Table II: Magnetic hyperfine splitting in the $^{229}\text{Th}^{87+}$ ion. The energy of the sublevels is in eV.

State I^π, F	Point nuclear magnetic dipole	Distributed nuclear magnetic dipole	
		Eqs. (8)-(9) of the present work	Mixing of the $F = 2$ levels
$5/2^+, 3$	0.0616	0.0597	0.0597
$5/2^+, 2$	-0.0862	-0.0836	-0.0841
$3/2^+, 2$	$E_{is} - 0.0104$	$E_{is} - 0.0097$	$E_{is} - 0.0092$
$3/2^+, 1$	$E_{is} + 0.0173$	$E_{is} + 0.0161$	$E_{is} + 0.0161$

Since two sublevels in the ions $^{229}\text{Th}^{89+,87+}$ has the same quantum number F , one has to take into account the mixing of these states [19, 22]:

$$\begin{aligned} |3/2^+, F=2\rangle' &= \sqrt{1-b^2}|3/2^+, F=2\rangle + b|5/2^+, F=2\rangle \\ |5/2^+, F=2\rangle' &= \sqrt{1-b^2}|5/2^+, F=2\rangle - b|3/2^+, F=2\rangle, \end{aligned}$$

where b is the mixing coefficient given by [62]

$$b = \frac{E_{|3/2^+, F=2\rangle'} - E_{|3/2^+, F=2\rangle}}{\sqrt{(E_{|3/2^+, F=2\rangle'} - E_{|3/2^+, F=2\rangle})^2 + E_{M1}^2}}.$$

It can be considered as a function of the energy E_{M1} related with the interaction of the electron and nuclear currents in the $M1$ electron transition in the ionic shell and the $M1$ nuclear transition between the ground and isomeric states. According to [18] the energy for the $E(M)L$ transition can be found as

$$\begin{aligned} E_{E(M)L}^2 &= 4\pi e^2 \frac{\omega_N^{2(L+1)}}{[(2L+1)!!]^2} \left(C_{ji1/2L0}^{j_f 1/2} \right)^2 \times \\ &\quad \langle f | m_L^{E(M)} | i \rangle^2 B(E(M)L, I_i \rightarrow I_f), \quad (12) \end{aligned}$$

where $C_{ji1/2L0}^{j_f 1/2}$ stands for the Clebsh-Gordon coefficients, $\langle f | m_L^{E(M)} | i \rangle$ is the electron matrix element and $B(E(M)L, I_i \rightarrow I_f)$ is the reduced probability of the nuclear transition [63].

In our case as a result of the $M1$ transition $|1s_{1/2}, 3/2^+\rangle \rightarrow |1s_{1/2}, 5/2^+\rangle$ in the $^{229}\text{Th}^{89+}$ ion or

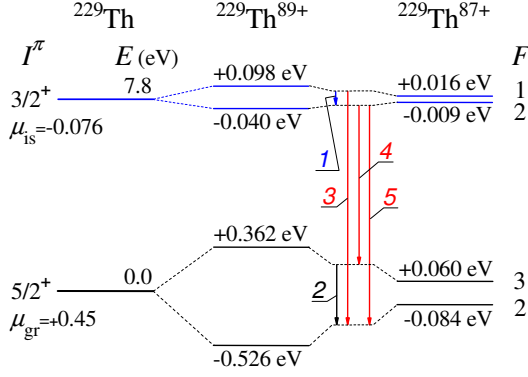


Figure 2: (color online). The magnetic hyperfine structure of the low energy doublet in $^{229}\text{Th}^{89+}$, $^{229}\text{Th}^{87+}$ and the $M1$ transitions between sublevels. The sublevels energy is counted from the energy of the level in the bare ^{229}Th nucleus.

the $M1$ transition $|2s_{1/2}, 3/2^+\rangle \rightarrow |2s_{1/2}, 5/2^+\rangle$ in the $^{229}\text{Th}^{87+}$ ion, Eq. (12) can be rewritten as

$$E_{M1}^2 = \frac{15}{2} \left(\frac{-2e^2 M_p}{3(M_p R_0)^2} \right)^2 |\langle f | m_1^M | i \rangle|^2 \times B_{W.u.}(M1, 3/2^+ \rightarrow 5/2^+). \quad (13)$$

Here $B_{W.u.}(M1, 3/2^+ \rightarrow 5/2^+)$ is the reduced probability of the nuclear isomeric transition in Weisskopf's units [64] and we have used that $B_{W.u.}(M1, 3/2^+ \rightarrow 5/2^+) = 3.0 \times 10^{-2}$ [34]. The electron matrix element of the $M1$ transition [18] reads as

$$\langle f | m_1^M | i \rangle = (\kappa_i + \kappa_f) \int_0^\infty h_1^{(1)}(\omega x) [g_i(x) f_f(x) + g_f(x) f_i(x)] x^2 dx,$$

where $\kappa = (l - j)(2j + 1)$, l and j are the quantum numbers of the electron orbital and total angular momenta, $h_1^{(1)}$ is the Hankel function of the first type.

We obtain $\langle 1s_{1/2} | m_1^M | 1s_{1/2} \rangle = -2.22 \times 10^{-4}$, $E_{M1} \simeq 0.4$ eV for the $^{229}\text{Th}^{89+}$ ion and $\langle 2s_{1/2} | m_1^M | 2s_{1/2} \rangle = -3.66 \times 10^{-5}$, $E_{M1} \simeq 0.07$ eV for the $^{229}\text{Th}^{87+}$ ion.

The new energies of the $F = 2$ sublevels are found as [62]

$$E_{|(4\mp 1)/2^+, F=2\rangle} = \frac{E_{|3/2^+, F=2\rangle} + E_{|5/2^+, F=2\rangle}}{2} \pm \frac{\sqrt{(E_{|3/2^+, F=2\rangle} - E_{|5/2^+, F=2\rangle})^2 + (2E_{M1})^2}}{2}, \quad (14)$$

The positions of the sublevels are shown in Fig. 2 and their energies are quoted in Tables I – II. The $^{229}\text{Th}^{89+}$ energies are in satisfactory correspondence with the data of [22]. The MHF splitting for $^{229}\text{Th}^{87+}$ shown in Fig. 2 are calculated for the first time.

VII. TRANSITIONS BETWEEN SUBLEVELS

In this section we calculate the probability of spontaneous transitions between the sublevels. According to [65] the radiative decay width of the $M1$ transition can be written as

$$\Gamma_{rad}(M1) = \frac{4}{3} \omega^3 \frac{1}{2F_i + 1} |\langle j_f I_f F_f | \mu_B \hat{\sigma} + \mu_{gr(is)} \mu_N \hat{I}/I + \hat{\mu}_{tr} \mu_N | j_i I_i F_i \rangle|^2. \quad (15)$$

Here $\mu_B \hat{\sigma}$ is the operator of the electron magnetic moment, $\mu_{gr(is)} \mu_N \hat{I}/I$ is the operator of the nuclear transition between the hyperfine components of the same level with spin I , and $\hat{\mu}_{tr} \mu_N$ is the operator of the transition between the ground and isomeric states.

In the case $j_i = j_f = 1/2$, $I_i = I_f = I_{gr(is)}$, for the transition between the hyperfine components $|F_i = I_{gr(is)} \pm 1/2\rangle \rightarrow |F_f = I_{gr(is)} \mp 1/2\rangle$ from Eq. (15) we obtain

$$\Gamma_{rad}(M1) = \frac{4}{3} e^2 \frac{\omega^3}{m^2} \frac{I_{gr(is)} + 1/2 \mp 1/2}{2I_{gr(is)} + 1} \times \left(1 + \frac{m}{M_p} \frac{\mu_{gr(is)}}{2I_{gr(is)}} \right)^2. \quad (16)$$

This expression coincides with Γ_{rad} for the $|F_i = I + 1/2\rangle \rightarrow |F_f = I - 1/2\rangle$ transition quoted in [66]. Clearly, the relative contribution from the operator $\mu_{gr(is)} \mu_N \hat{I}/I$ given in the second term in the parentheses of Eq. (16), is small and will be omitted below.

The probability associated with the operator $\hat{\mu}_{tr} \mu_N$ is negligibly small for both ions. This is a consequence of the states mixing. The effect was already mentioned in [22] for the $^{229}\text{Th}^{89+}$ ion. Although the coefficient b is several times smaller for the $^{229}\text{Th}^{87+}$ ion ($b_{87+} = 0.0083$ versus $b_{89+} = 0.048$) it is nevertheless enough for enabling the noticeable transitions between the hyperfine sublevels through the electron spin-flip transition.

The calculated radiative decay widths Γ_{rad} and the associated transition times τ are given in Table III. Probabilities for the transitions 1 and 2 have been computed by means of Eq. (16). For the transitions 3 and 4 the value from Eq. (16) was further multiplied by b^2 . The transition 5 involves the electron spin-flip transitions $|I_i = F \mp 1/2, F\rangle \rightarrow |I_f = F \pm 1/2, F\rangle$ (due to the mixing of the $F = 2$ states) and its radiative width is calculated according to the equation

$$\Gamma_{rad}(M1) = \frac{4}{3} e^2 \frac{\omega^3}{m^2} \frac{b^2(1 - b^2)}{4F(F + 1)}, \quad (17)$$

which can be derived from (15).

The results for $^{229}\text{Th}^{89+}$ are in fair correspondence with the data of [22]. (Notice that in Ref. [22], as in other works up to 2007, it was assumed that $E_{is} = 3.5$ eV.)

To demonstrate the increased probability of the transitions 3, 4 and 5, we compare their widths with the

Table III: Radiative widths Γ_{rad} and times $\tau = \ln(2)/\Gamma_{rad}$ for the transitions between the sublevels of MHF structure in $^{229}\text{Th}^{89+}$ and $^{229}\text{Th}^{87+}$.

Transition		$^{229}\text{Th}^{89+}$		$^{229}\text{Th}^{87+}$	
N	$I_i^\pi, F_i \rightarrow I_f^\pi, F_f$	Γ_{rad} (eV)	τ	Γ_{rad} (eV)	τ
1	$3/2^+, 1 \rightarrow 3/2^+, 2$	6.2×10^{-17}	7.4 s	3.8×10^{-19}	20 min
2	$5/2^+, 3 \rightarrow 5/2^+, 2$	1.1×10^{-14}	42 ms	4.6×10^{-17}	10 s
3	$3/2^+, 1 \rightarrow 5/2^+, 2$	3.2×10^{-14}	14 ms	8.0×10^{-16}	0.57 s
4	$3/2^+, 2 \rightarrow 5/2^+, 3$	2.2×10^{-14}	21 ms	7.6×10^{-16}	0.61 s
5	$3/2^+, 2 \rightarrow 5/2^+, 2$	2.0×10^{-15}	0.23 s	5.2×10^{-17}	8.7 s

radiative width $\Gamma_{rad}(3/2^+ \rightarrow 5/2^+)$ for the $M1$ isomeric transition in the naked nucleus ^{229}Th . In that case only the operator $\hat{\mu}_{tr}\mu_N$ remains in Eq. (15). We express its matrix element in terms of the reduced probability of the nuclear transition:

$$B(M1; I_i \rightarrow I_f) = \frac{3}{4\pi} \frac{|\langle I_f || \hat{\mu}_{tr} || I_i \rangle|^2}{2I_i + 1}.$$

We then arrive at $B(M1; 3/2^+ \rightarrow 5/2^+) = (45/8\pi)\mu_N^2 B_{W.u.}(M1, 3/2^+ \rightarrow 5/2^+) = 5.37 \times 10^{-2}\mu_N^2$. (The factor $3/4\pi$ is accounted for by the differences in the definition of the transition operators in the atomic [65] and nuclear [59] physics.) As a result we have $\Gamma_{rad}(3/2^+ \rightarrow 5/2^+) = 3 \times 10^{-19}$ eV, which corresponds to $\tau = 26$ min.

VIII. CONCLUSION

In conclusion, the calculation of the magnetic hyperfine structure of the ground state doublet (the ground $5/2^+(0.0)$ and the low energy $3/2^+(7.8$ eV) isomeric states) in the highly ionized ions $^{229}\text{Th}^{89+}$ and $^{229}\text{Th}^{87+}$ have been performed.

We have demonstrated that in comparison with the point nucleus model the Bohr-Weisskopf effect (finite distribution of nuclear magnetization) decreases the hyperfine splitting by 3% for the ground state and by 6% for the isomeric state. The energies of the sublevels have been calculated by taking into account the mixing of states with the same quantum number $F = 2$. As a result of mixing the energy difference between two F states increases by 0.04 eV in $^{229}\text{Th}^{89+}$ and 0.001 eV in $^{229}\text{Th}^{87+}$.

The mixing of states (with the coefficients $b_{89+} = 0.048$ and $b_{87+} = 0.0083$) has been taken into account in the estimation of the probability of spontaneous transitions. We have found that even in the $^{229}\text{Th}^{87+}$ ion the mixing leads to a large increase of the probability of radiative transitions. The transitions therefore are caused mainly by a small admixture of other quantum states.

It is worth noting that the Bohr-Weisskopf effect completely compensates the energy shift of the $|5/2^+, F = 2\rangle$ level in the $^{229}\text{Th}^{89+, 87+}$ ions, caused by the mixing. It also has profound influence on the energy positions of the states with $F = 3$ and $F = 1$. Therefore, the data on the hyperfine splittings can be used for precise determination of the magnetic moments of the nuclear $5/2^+(0.0)$ and $3/2^+(7.8$ eV) states.

Our findings can be useful for experiments with highly ionized ^{229}Th ions in the storage ring of accelerator complex.

IX. ACKNOWLEDGMENTS

One of the authors (E.T.) is grateful to Prof. S. Wycech, who has drawn our attention to the importance of the calculation of the MHF splitting in the $^{229}\text{Th}^{87+}$ ion for experimental studies in the accelerator storage ring.

This research was supported by a grant of Russian Science Foundation (project No 16-12-00001).

-
- | | |
|---|---|
| <p>[1] B. R. Beck, J. A. Becker, P. Beiersdorfer, G. V. Brown, K. J. Moody, J. B. Wilhelmy, F. S. Porter, C. A. Kilbourne, and R. L. Kelley, Phys. Rev. Lett. 98, 142501 (2007).</p> <p>[2] B. R. Beck, J. A. Becker, P. Beiersdorfer, G. V. Brown, K. J. Moody, J. B. Wilhelmy, F. S. Porter, C. A. Kilbourne and R. L. Kelley, Report LLNL-PROC-415170.</p> <p>[3] C. W. Reich and R. G. Helmer, Phys. Rev. Lett. 64, 271 (1990).</p> <p>[4] R. G. Helmer and C. W. Reich, Phys. Rev. C 49, 1845 (1994).</p> <p>[5] G. M. Irwin and K. H. Kim, Phys. Rev. Lett. 79, 990 (1997).</p> <p>[6] D. S. Richardson, D. M. Benton, D. E. Evans, J. A. R. Griffith, and G. Tungeate, Phys. Rev. Lett. 80, 3206 (1998).</p> <p>[7] R. W. Shaw, J. P. Young, S. P. Cooper, and O. F. Webb, Phys. Rev. Lett. 82, 1109 (1999).</p> | <p>[8] S. B. Utter, P. Beiersdorfer, A. Barnes, R. W. Lougheed, J. R. Crespo Lopez-Urrutia, J. A. Becker, and M. S. Weiss, Phys. Rev. Lett. 82, 505 (1999).</p> <p>[9] H. Kikunaga, Y. Kasamatsu, K. Takamiya, T. Mitsugashira, M. Hara, T. Ohtsuki, H. Yuki, A. Shinohara, S. Shibata, N. Kinoshita, A. Yokoyama, and T. Nakanishi. Research Rep. Lab. Nucl. Sci., Tohoku University, 38, 25 (2005).</p> <p>[10] C. J. Campbell, A. V. Steele, L. R. Churchill, M. V. DePalatis, D. E. Naylor, D. N. Matsukevich, A. Kuzmich, and M. S. Chapman, Phys. Rev. Lett. 102, 233004 (2009).</p> <p>[11] C. J. Campbell, A. G. Radnaev, and A. Kuzmich, Phys. Rev. Lett. 106, 223001 (2011).</p> <p>[12] C. J. Campbell, A. G. Radnaev, A. Kuzmich, V. A. Dzuba, V. V. Flambaum, and A. Derevianko, Phys. Rev. Lett. 108, 120802 (2012).</p> <p>[13] M. P. Hehlen, R. R. Greco, W. G. Rellergert, S. T. Sulli-</p> |
|---|---|

- van, D. DeMille, R. A. Jackson, E. R. Hudson, and J. R. Torgerson, *J. Luminescence* **49**, 133 (2013).
- [14] J. Jeet, C. Schneider, S. T. Sullivan, W. G. Rellergert, S. Mirzadeh, A. Cassanho, H. P. Jenssen, E. V. Tkalya, and E. R. Hudson, *Phys. Rev. Lett.* **114**, 253001 (2015).
- [15] A. Yamaguchi, M. Kolbe, H. Kaser, T. Reichel, A. Gottwald, and E. Peik, *New J. Phys.* **17**, 053053 (2015).
- [16] L. von der Wense, B. Seiferle, M. Laatiaoui, J. B. Neumayr, H.-J. Maier, H.-F. Wirth, C. Mokry, J. Runke, K. Eberhardt, C. E. Dullmann, et al., *Nature* **533**, 47 (2016).
- [17] V. F. Strizhov and E. V. Tkalya, *Sov. Phys. JETP* **72**, 387 (1991).
- [18] E. V. Tkalya, *Nucl. Phys. A* **539**, 209 (1992).
- [19] S. Wycech and J. Zylicz, *Acta Phys. Pol. B* **24**, 637 (1993).
- [20] E. V. Tkalya, V. O. Varlamov, V. V. Lomonosov, and S. A. Nikulin, *Phys. Scr.* **53**, 296 (1996).
- [21] A. M. Dykhne, N. V. Eremin, and E. V. Tkalya, *JETP Lett.* **64**, 345 (1996).
- [22] F. F. Karpeshin, S. Wycech, I. M. Band, M. B. Trzhaskovskaya, M. Pfutzner, and J. Zylicz, *Phys. Rev. C* **57**, 3085 (1998).
- [23] A. M. Dykhne and E. V. Tkalya, *JETP Lett.* **67**, 251 (1998).
- [24] A. M. Dykhne and E. V. Tkalya, *JETP Lett.* **67**, 549 (1998).
- [25] E. V. Tkalya, *JETP Lett.* **71**, 311 (2000).
- [26] E. V. Tkalya, A. N. Zherikhin, and V. I. Zhudov, *Phys. Rev. C* **61**, 064308 (2000).
- [27] E. V. Tkalya, *Physics-Uspekhi* **46**, 315 (2003).
- [28] V. V. Flambaum, *Phys. Rev. Lett.* **97**, 092502 (2006).
- [29] J. C. Berengut, V. A. Dzuba, V. V. Flambaum, and S. G. Porsev, *Phys. Rev. Lett.* **102**, 210801 (2009).
- [30] E. Litvinova, H. Feldmeier, J. Dobaczewski, and V. Flambaum, *Phys. Rev. C* **79**, 064303 (2009).
- [31] E. V. Tkalya, *Phys. Rev. Lett.* **106**, 162501 (2011).
- [32] G. A. Kazakov, A. N. Litvinov, V. I. Romanenko, L. P. Yatsenko, A. V. Romanenko, M. Schreitzl, G. Winkler, and T. Schumm, *New J. Phys.* **14**, 083019 (2012).
- [33] K. Beloy, *Phys. Rev. Lett.* **112**, 062503 (2014).
- [34] E. V. Tkalya, C. Schneider, J. Jeet, and E. R. Hudson, *Phys. Rev. C* **92**, 054324 (2015).
- [35] V. V. Flambaum and R. B. Wiringa, *Phys. Rev. C* **79**, 034302 (2009).
- [36] V. A. Dzuba and V. V. Flambaum, *Phys. Rev. A* **81**, 034501 (2010).
- [37] L. V. Skripnikov, A. N. Petrov, A. V. Titov, and V. V. Flambaum, *Phys. Rev. Lett.* **113**, 263006 (2014).
- [38] V. V. Flambaum, arXiv:1603.05753v1 (2016).
- [39] S. G. Porsev and V. V. Flambaum, *Phys. Rev. A* **81**, 042516 (2010).
- [40] E. V. Tkalya, *JETP Lett.* **55**, 211 (1992).
- [41] S. G. Porsev, V. V. Flambaum, E. Peik, and C. Tamm, *Phys. Rev. Lett.* **105**, 182501 (2010).
- [42] E. Peik and C. Tamm, *Europhys. Lett.* **61**, 181 (2000).
- [43] W. G. Rellergert, D. DeMille, R. R. Greco, M. P. Hehlen, J. R. Torgerson, and E. R. Hudson, *Phys. Rev. Lett.* **104**, 200802 (2010).
- [44] E. Peik and M. Okhapkin, *C. R. Phys.* **16**, 516 (2015).
- [45] E. V. Tkalya and L. P. Yatsenko, *Laser Phys. Lett.* **10**, 105808 (2013).
- [46] H. Geissel, K. Beckert, F. Bosch, et al., *Phys. Rev. Lett.* **68**, 3412 (1992).
- [47] I. Klaft, S. Borneis, T. Engel, et al., *Phys. Lett. Lett.* **73**, 2425 (1994).
- [48] T. Radon, T. Kerscher, B. Schlitt, et al., *Phys. Rev. Lett.* **78**, 4701 (1997).
- [49] X. Ma, W. Q. Wen, Z. K. Huang, H. B. Wang, Y. J. Yuan, M. Wang, Z. Y. Sun, L. J. Mao, J. C. Yang, H. S. Xu, et al., *Phys. Scr.* **T166**, 014012 (2015).
- [50] A. Abragam, *The Principles of Nuclear Magnetism* (Clarendon Press, Oxford, England, 1961).
- [51] A. V. Nikolaev, D. Lamoén and B. Partoens, arXiv:1503.05827v2 (2015).
- [52] A. V. Nikolaev, The FLAPW-Moscow code [registration number 2015616990 (Russia) from 26/06/2015].
- [53] P. A. M. Dirac, *Proc. Camb. Philos. Soc.* **26**, 376 (1930).
- [54] J. P. Perdew and Y. Wang, *Phys. Rev. B* **45**, 13244 (1992).
- [55] J. P. Perdew, K. Burke, and M. Ernzerhof, *Phys. Rev. Lett.* **77**, 3865 (1996).
- [56] J. P. Perdew, K. Burke, and M. Ernzerhof, *Phys. Rev. Lett.* **78**, 1396 (1997).
- [57] A. Bohr and V. F. Weisskopf, *Phys. Rev.* **77**, 94 (1950).
- [58] M. Le Bellac, *Nucl. Phys.* **40**, 645 (1963).
- [59] A. Bohr and B. R. Mottelson, *Nuclear Structure. Vol. II: Nuclear Deformations.* (World Scientific, London, 1998).
- [60] D. A. Varshalovich, A. N. Moskalev, and V. K. Khersonskii, *Quantum Theory of Angular Momentum* (World Scientific Publ., London, 1988).
- [61] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (National Bureau of Standards, Washington, D.C., 1964).
- [62] A. S. Davydov, *Quantum Mechanics* (Pergamon Press, Oxford, England, 1965).
- [63] A. Bohr and B. R. Mottelson, *Nuclear Structure. Vol. I: Single-Particle Motion.* (World Scientific, London, 1998).
- [64] J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley and Sons, Inc., New York, 1952).
- [65] V. B. Berestetskii, E. M. Lifschitz, and L. P. Pitaevskii, *Quantum Electrodynamics* (Pergamon Press, Oxford, England, 1982).
- [66] R. Winston, *Phys. Rev.* **129**, 2766 (1963).